PETRA ŽIGERT PLETERŠEK, University of Maribor, Slovenia
Topological indices of unsaturated hydrocarbons

Hydrocarbons are modeled with simple graphs but in the case of unsaturated hydrocarbons with multiple bonds the corresponding graphs should be multigraphs. There is some ambiguity in modeling such graphs, and consequently in the calculation of certain topological indices. We introduce a model of edge-weighted graphs where distances in a graph are defined in three different ways using the topological distance, the relative topological distance and the relative distance (actual lengths of bonds). The regression analysis on the obtained weighted Wiener indices is performed and gives a good model for the prediction of boiling points of alkenes and alkadienes.